NERL Publication Report
April 1 – April 8, 2019

Published Articles & Reports

[HYPERLINK "https://doi.org/10.1016/j.atmosenv.2019.04.004 "]	Zhang, S., Xing, J., Sarwar, G., Ge, Y., He, H., Duan, F., Zhao, Y., He, K., Zhu, L., Chu, B. (2019) Parameterization of heterogeneous reaction of SO2 to sulfate on dust with coexistence of NH3 and NO2 under different humidity conditions. ATMOSPHERIC ENVIRONMENT. Available Online, https://doi.org/10.1016/j.atmosenv.2019.04.004	CED-AMDB	Peer Reviewed	ACE AIMS-1.4

Impact / Purpose Statement
Current CMAQ and other air quality models cannot predict elevated wintertime observed sulfate concentration in China. Previous investigators have examined the impact of heterogeneous conversion of SO2 into sulfate with various types of parameterizations. In this study, an uptake coefficient for heterogeneous oxidation of SO2 was developed using experimental results that approximate the haze conditions in China which was then implemented into the CMAQ model. Simulation results suggest that this new parameterization can improve model performance in the simulation of wintertime sulfate concentration by 6.6% for Beijing. The simulated maximum growth rate of SO42- during heavy pollution period increased from 0.97μg/m3/h to 10.11μg/m3/h. The heterogeneous oxidation of SO2 in the presence of NH3 can contribute up to 23% of the sulfate concentration during heavy pollution periods.

Product Description / Abstract
Sulfate plays an important role in atmospheric haze in China, which has received considerable attention in recent years. Various types of parameterization methods and heterogeneous oxidation rates of SO2 have been used in previous studies. However, properly representing heterogeneous sulfate formation in air quality models remains a big challenge. In this study, we quantified the heterogeneous oxidation reaction using experimental results that approximate the haze conditions in China. Firstly, a series of experiments were conducted to investigate the heterogeneous uptake of SO2 with different relative humidity (RH) levels and the presence of NH3 and NO2 on natural dust surfaces. Then the uptake coefficients for heterogeneous oxidation of SO2 to sulfate at different RH under NH3 and NO2 coexistence were parameterized based on the experimental results and implemented in the Community Multiscale Air Quality modeling system (CMAQ). Simulation results suggested that this new parameterization improved model performance by 6.6% in the simulation of wintertime sulfate concentrations for Beijing. The simulated maximum growth rate of SO42− during a heavy pollution period increased from 0.97 μg m−3 h−1 to 10.11 μg m−3 h−1. The heterogeneous oxidation of SO2 in the presence of NH3 contributed up to 23% of the sulfate concentration during heavy pollution periods.

Submitted

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)

Ex. 5 Deliberative Process (DP)